

Fermi surfaces of iron-pnictide high- T_c superconductors from the limit of local magnetic moments

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Abstract

A 2-orbital t - J model over the square lattice that describes low-energy electronic excitations in iron-pnictide high- T_c superconductors is analyzed with Schwinger-boson-slave-fermion mean field theory and by exact numerical diagonalization on a finite system. When inter-orbital hole hopping is suppressed, a quantum critical point (QCP) is identified that separates a commensurate spin-density wave (cSDW) state at strong Hund's rule coupling from a hidden half-metal state at weak Hund's rule coupling. Low-energy spinwaves that disperse anisotropically from cSDW momenta are predicted at the QCP. Nested Fermi surfaces similar to those observed experimentally in iron-pnictide materials are also predicted in such case.

I. INTRODUCTION

High-temperature superconductivity in iron-pnictide materials is achieved by injecting charge carriers into stoichiometric parent compounds that show commensurate spin-density wave (cSDW) order over a tetragonal lattice of iron atoms[1][2]. The charge carriers in these systems have predominantly iron $3d$ -orbital character[3][4][5], and they exist at two-dimensional (2D) hole-type and electron-type Fermi surface pockets centered, respectively, at zero 2D momentum and at the 2D cSDW momenta $(h/2a)\hat{\mathbf{x}}(\hat{\mathbf{y}})$ [6][7][8]. Here, a is the iron 2D lattice constant. Density functional theory (DFT) calculations correctly account for the Fermi surfaces that are also observed in the cSDW[9], but they predict an ordered moment of approximately 2 Bohr magnetons (μ_B) that is large compared to measured values that can be as low as $0.3 \mu_B$ [2]. Frustrated 2D Heisenberg models that assume local magnetic moments at the iron atoms can account for the weak cSDW observed in parent compounds, on the other hand[10][11][12][13][14]. They cannot predict the observed Fermi surface pockets, however, because local-moment magnets are Mott insulators.

Below, we introduce mobile holes into a two-orbital local-moment model for frustrated magnetism that successfully describes the weak cSDW nature of iron-pnictide systems[14]. Exact diagonalization of one hole that hops over a square lattice of iron atoms in a single layer obtains a robust cSDW groundstate at $1/2$ the cSDW momenta when Hund's rule is obeyed (cf. ref. [15]). Both the exact and a mean-field analysis find that two Fermi surface hole pockets centered at zero 2D momentum can emerge when Hund's rule is violated, at sufficiently weak inter-orbital hopping of electrons. The ground state in question is the half-metal state with antiferromagnetic order across the $3d_{(x+iy)z}$ and $3d_{(x-iy)z}$ orbitals of the iron atom[14]. Proximity to a quantum critical point (QCP) that separates the hidden half-metal at weak Hund's coupling from a cSDW metal[16] at strong Hund's coupling results in weak cSDW order and in low-energy spin-wave excitations at cSDW wave numbers. The latter disperse in a manner that is consistent with inelastic neutron scattering (INS) measurements in iron-pnictide metals[17][18]. The critical spinwaves in turn result in nested Fermi surface pockets that are centered at cSDW wave numbers, in agreement with angle-resolved photoemission (ARPES) on iron-pnictide metals[7]. These have mixed electron-type and hole-type character, however, which is a feature that has also been seen in ARPES studies of iron-pnictide metals[8].

II. 2-ORBITAL t - J MODEL: MEAN FIELD THEORY AND EXACT RESULTS

We shall now show that a hidden half-metal groundstate emerges from the following two-orbital t - J model over the square lattice, where double occupancy at a site-orbital is strictly forbidden:

$$H = - \sum_{\langle i,j \rangle} \sum_{\alpha,\beta} \sum_s (t_1^{\alpha,\beta} \tilde{c}_{i,\alpha,s}^\dagger \tilde{c}_{j,\beta,s} + \text{h.c.}) + \frac{1}{2} J_0 \sum_i \left[\sum_{\alpha} \mathbf{S}_{i,\alpha} \right]^2 + \sum_{\langle i,j \rangle} \sum_{\alpha,\beta} J_1^{\alpha,\beta} \mathbf{S}_{i,\alpha} \cdot \mathbf{S}_{j,\beta} + \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha,\beta} J_2^{\alpha,\beta} \mathbf{S}_{i,\alpha} \cdot \mathbf{S}_{j,\beta}. \quad (1)$$

Above, $\mathbf{S}_{i,\alpha}$ is the spin operator that acts on the spin $s_0 = 1/2$ state of the $3d_{(x+iy)z}$ ($d+$) or $3d_{(x-iy)z}$ ($d-$) orbital, $\alpha = 0$ or 1 , in the iron atom at site i . The latter runs over the square lattice of iron atoms that make up an isolated layer. The former basis of $d\pm$ orbitals is the least localized one (cf. ref. [19]), which maximizes the Hund's coupling, $-J_0$. It therefore minimizes the Hund's rule exchange energy in the 2-orbital t - J model (1). Nearest neighbor and next-nearest neighbor Heisenberg exchange across the links $\langle i,j \rangle$ and $\langle\langle i,j \rangle\rangle$ is controlled by the exchange coupling constants $J_1^{\alpha,\beta}$ and $J_2^{\alpha,\beta}$, respectively. These are necessarily isotropic over the $d\pm$ orbital basis. Correlated hopping of an electron in orbital α to a neighboring unoccupied orbital β is controlled by the hopping matrix element $t_1^{\alpha,\beta}$. The Heisenberg model that corresponds to (1) in the absence of charge carriers possesses a QCP at large s_0 that separates a cSDW at strong Hund's coupling from a hidden ferromagnet that shows $\nearrow_{d+} \searrow_{d-}$ spin order at weak Hund's coupling if off-diagonal frustration exists[14]: e.g. $J_1^\parallel = 0$, $J_1^\perp > 0$, and $J_2^\parallel = J_2^\perp > 0$. Here the superscripts \parallel and \perp refer to the relationship between the orbital indices α and β . Recent DFT calculations show that the superposition of direct ferromagnetic exchange with super-exchange across nearest-neighbor iron atoms can result in the cancellation $J_1^\parallel = 0$ [4]. The remaining positive exchange coupling constants are assumed to be due to the super-exchange mechanism[10][20].

Let us now turn off inter-orbital hopping: $t_1^\perp = 0$. Notice that antiferromagnetic order across the $d+$ and $d-$ orbitals then remains intact in the presence of mobile holes[14]. This is a classical picture for a half-metal groundstate that shows $\nearrow_{d+} \searrow_{d-}$ spin order. To describe it, we adopt the Schwinger-boson (b) slave-fermion (f) representation for the correlated electron[15][21]: $\tilde{c}_{i,\alpha,s} = b_{i,\alpha,s} f_{i,\alpha}^\dagger$ and $\mathbf{S}_{i,\alpha} = (1/2) \sum_{s,s'} f_{i,\alpha} b_{i,\alpha,s}^\dagger \boldsymbol{\sigma}_{s,s'} b_{i,\alpha,s'} f_{i,\alpha}^\dagger$, with the constraint

$$2s_0 = b_{i,\alpha,\uparrow}^\dagger b_{i,\alpha,\uparrow} + b_{i,\alpha,\downarrow}^\dagger b_{i,\alpha,\downarrow} + f_{i,\alpha}^\dagger f_{i,\alpha} \quad (2)$$

imposed at each site-orbital to exclude double occupancy. From here on we set $\hbar = 1$. Following Arovas and Auerbach[22], we next rotate about the spin y axis by an angle π on one of the antiferromagnetic sublattices in order to decouple the spins: $b_{i,0,\uparrow} \rightarrow -b_{i,0,\downarrow}$ and $b_{i,0,\downarrow} \rightarrow b_{i,0,\uparrow}$. Again following these authors, we now define mean fields that are set by the pattern of ferromagnetic (\parallel) versus antiferromagnetic (\perp) pairs of neighboring spins: $Q_0^\perp = \langle b_{i,\alpha,s} b_{i,\beta,s} \rangle$, $Q_{1(2)}^\parallel = \langle b_{i,\alpha,s}^\dagger b_{j,\alpha,s} \rangle$ and $Q_{1(2)}^\perp = \langle b_{i,\alpha,s} b_{j,\beta,s} \rangle$ for (next) nearest-neighbor links, where $\alpha \neq \beta$. We add to that list the mean field $P_1^\parallel = \frac{1}{2} \langle f_{i,\alpha}^\dagger f_{j,\alpha} \rangle$ for nearest-neighbor hopping of holes within the same orbital. The mean-field approximation for the t - J model Hamiltonian (1) then has the form $H_{MF} = H_0[Q, P] + H_b + H_f$, where $H_0[Q, P]$ consolidates the bilinear terms among the mean fields, where

$$H_b = \frac{1}{2} \sum_k \sum_s \{ \Omega_\parallel(k) [b_s^\dagger(k) b_s(k) + b_s(-k) b_s^\dagger(-k)] + \Omega_\perp(k) [b_s^\dagger(k) b_s^\dagger(-k) + b_s(-k) b_s(k)] \}$$

is the Hamiltonian for free Schwinger bosons, with

$$\begin{aligned} \Omega_\parallel(k) &= \delta\lambda + \sum_{n=0,1,2} z_n J_n'^\perp Q_n^\perp - 4(J_1'^\parallel Q_1^\parallel + 2t_1^\parallel P_1^\parallel)[1 - \gamma_1(\mathbf{k})] - 4J_2'^\parallel Q_2^\parallel[1 - \gamma_2(\mathbf{k})] \\ \Omega_\perp(k) &= -e^{ik_0} \sum_{n=0,1,2} z_n J_n'^\perp Q_n^\perp \gamma_n(\mathbf{k}), \end{aligned}$$

and where $H_f = \sum_k \varepsilon_f(k) f^\dagger(k) f(k)$ is the Hamiltonian for free slave fermions, with $\varepsilon_f(k) = 8t_1^\parallel Q_1^\parallel \gamma_1(\mathbf{k}) - \mu$. Above, $k = (k_0, \mathbf{k})$ is the 3-momentum for these excitations, with corresponding destruction operators $b_s(k) = \mathcal{N}^{-1/2} \sum_{\alpha=0}^1 \sum_i e^{i(k_0\alpha + \mathbf{k} \cdot \mathbf{r}_i)} b_{i,\alpha,s}$ and $f(k) = \mathcal{N}^{-1/2} \sum_{\alpha=0}^1 \sum_i e^{i(k_0\alpha + \mathbf{k} \cdot \mathbf{r}_i)} f_{i,\alpha}$. Here $k_0 = 0, \pi$ represent even and odd superpositions of the $d\pm$ orbitals, while $\mathcal{N} = 2N_{\text{Fe}}$ denotes the number of sites-orbitals on the square lattice of iron atoms. Also above, $z_0 = 1$ and $z_{1(2)} = 4$, $\gamma_0(\mathbf{k}) = 1$ and $\gamma_{1(2)}(\mathbf{k}) = \frac{1}{2}(\cos k_{x(+)}a + \cos k_{y(-)}a)$, where $k_\pm = k_x \pm k_y$, while $\delta\lambda$ is the boson chemical potential that enforces the constraint against double occupancy (2) on *average* over the bulk of the system. The concentration of mobile holes per site-orbital, x , sets the chemical potential of the slave fermions, μ . Last, the effect of mobile holes on the Heisenberg spin-exchange is accounted for by the effective exchange coupling constants[21] $J' = (1 - x)^2 J$.

The solution to the above mean field theory is achieved by making the standard Bogoliubov transformation of the boson field, $b_s(k) = (\cosh \theta_k) \beta_s(k) + (\sinh \theta_k) \beta_s^\dagger(-k)$, with $\cosh 2\theta = \Omega_\parallel / \omega_b$ and $\sinh 2\theta = -\Omega_\perp / \omega_b$, where $\omega_b = (\Omega_\parallel^2 - \Omega_\perp^2)^{1/2}$ is the energy eigenvalue of the (β) boson. Enforcing the constraint against double occupancy (2) on average then

yields the principal mean field equation[22]

$$s_0 + \frac{1}{2} - \frac{1}{2}x = \mathcal{N}^{-1} \sum_k (\cosh 2\theta_k)(n_B[\omega_b(k)] + \frac{1}{2}), \quad (3)$$

where n_B denotes the Bose-Einstein distribution. Ideal Bose-Einstein condensation (BEC) into the two lowest-energy states at $\mathbf{k} = 0$ occurs as temperature $T \rightarrow 0$, in which case $\delta\lambda \rightarrow 0$. The remaining self-consistent equations for the Schwinger-boson mean fields are

$$\begin{aligned} Q_n^\parallel &= \mathcal{N}^{-1} \sum_k \gamma_n(\mathbf{k})(\cosh 2\theta_k)(n_B[\omega_b(k)] + \frac{1}{2}) \quad \text{and} \\ Q_n^\perp &= \mathcal{N}^{-1} \sum_k \gamma_n(\mathbf{k})e^{ik_0}(\sinh 2\theta_k)(n_B[\omega_b(k)] + \frac{1}{2}). \end{aligned}$$

After comparison with (3), ideal BEC as $T \rightarrow 0$ implies the unique value $Q = s_0$ for all five of these mean fields in the large- s_0 limit. Last, the self-consistent mean field equation for intra-orbital hole hopping is $P_1^\parallel = \mathcal{N}^{-1} \sum_{\mathbf{k}} \gamma_1(\mathbf{k})n_F[\varepsilon_f(\mathbf{k})]$, where n_F is the Fermi distribution function. We henceforth assume a hole band at low doping, $t_1^\parallel < 0$ and $x \ll 1$, which implies two degenerate circular Fermi surfaces centered at zero 2D momentum with Fermi wave vector $k_F a = (4\pi x)^{1/2}$. This yields the amplitude $P_1^\parallel = x/2$ for intra-orbital hole hopping. Inspection of the spectrum for Schwinger bosons, $\omega_b(\mathbf{k})$, yields a spin gap at cSDW wave numbers $(\pi/a)\hat{\mathbf{x}}(\hat{\mathbf{y}})$ equal to

$$\Delta_{cSDW} = (1-x)^2(2s_0)[(4J_2^\perp - J_{0c})(J_0 - J_{0c})]^{1/2}, \quad (4)$$

where $-J_{0c} = 2(J_1^\perp - J_1^\parallel) - 4J_2^\parallel - (1-x)^{-2}s_0^{-1}2t_1^\parallel x$ is the critical Hund's coupling at which $\Delta_{cSDW} \rightarrow 0$. Notice that intra-orbital hole hopping stabilizes the hidden half-metal state. We therefore propose (i) that the normal state of iron-pnictide superconductors is described by the present hidden half-metal state, and (ii) that the cSDW/superconductor transition that these systems commonly exhibit[2][7] is controlled by the QCP at Hund's coupling $-J_{0c}$. The linear increase of $-J_{0c}$ with the concentration of holes x implies a charge-carrier-poor cSDW and a charge-carrier-rich superconductor, which is consistent with experiment.

Transverse dynamical spin correlations are obtained directly from the above Schwinger-boson-slave-fermion mean field theory. In particular, we have

$$\langle S_{x(y)} S_{x(y)} \rangle|_{k_0, \mathbf{k}, \omega} = \frac{1}{2}(1-x)^2 [G_b * G_b^* + (-)F_b * F_b^*]|_{\pi(0)+k_0, \mathbf{k}, \omega},$$

where $iG_b(k, \omega) = \langle b_s(k, \omega)b_s^\dagger(k, \omega) \rangle$ and $iF_b(k, \omega) = \langle b_s(k, \omega)b_s(-k, -\omega) \rangle$ are the regular and the anomalous Greens functions for the Schwinger bosons, and where the notation

$f * g$ denotes a convolution in frequency and momentum. This yields an Auerbach-Arovas expression for the dynamical spin correlator at $T > 0$ [23]. It is easily evaluated in the zero-temperature limit, where ideal BEC of the Schwinger bosons into the doubly degenerate $\mathbf{k} = 0$ ground state occurs. It contributes to half of the net transverse spin correlator, which in this limit and at large s_0 reads

$$i\langle \mathbf{S}_\perp \cdot \mathbf{S}_\perp \rangle|_{k,\omega} = (1-x)^2 s_0 (\Omega_+/\Omega_-)^{1/2} ([\omega_b(k) - \omega]^{-1} + [\omega_b(k) + \omega]^{-1}). \quad (5)$$

Here, $\Omega_\pm = \Omega_\parallel \pm \Omega_\perp$. The above dynamical spin correlator coincides with the transverse spin susceptibility, $\chi_\perp(k, \omega)$, in the present zero-temperature limit by the fluctuation-dissipation theorem. Observe now that $\Omega_-(\pi, \mathbf{k})$ and $\Omega_+(0, \mathbf{k})$ both vanish at $\mathbf{k} = 0$ in general, while $\Omega_-(0, \mathbf{k})$ and $\Omega_+(\pi, \mathbf{k})$ both vanish at cSDW wave vectors $\mathbf{k} = (\pi/a)\hat{\mathbf{x}}(\hat{\mathbf{y}})$ at the QCP [14]. The identity $\omega_b = (\Omega_- \Omega_+)^{1/2}$ then ultimately yields that spinwaves at zero 2D momentum disperse isotropically as $\omega_b(\mathbf{k}) = v_0|\mathbf{k}|$, while those at cSDW wave numbers disperse anisotropically as

$$\omega_b(\mathbf{k}) = [v_0^2(k_l - \pi/a)^2 + v_0^2(k_t/\gamma_{cSDW})^2 + \Delta_{cSDW}^2]^{1/2}. \quad (6)$$

(See fig. 1a.) Here, k_l and k_t are the longitudinal and the transverse components of \mathbf{k} with respect to the cSDW wave number. The longitudinal spin-wave velocity is

$$v_0 = 2s_0 a (1-x)^2 ([J_1^\perp - J_1^\parallel(x) + 2(J_2^\perp - J_2^\parallel)] \cdot [\frac{1}{2}J_0 + 2J_1^\perp + 2J_2^\perp])^{1/2} \quad (7)$$

and the anisotropy parameter is

$$\gamma_{cSDW} = ([2(J_2^\parallel + J_2^\perp) + J_1^\parallel(x) + J_1^\perp]/[2(J_2^\parallel + J_2^\perp) - J_1^\parallel(x) - J_1^\perp])^{1/2}, \quad (8)$$

which is greater than unity. Here $J_1^\parallel(x) = J_1^\parallel + (1-x)^{-2} s_0^{-1} t_1^\parallel x$. Study of the spectral weights in expression (5) for $\chi_\perp(k, \omega)$ then yields that the former spinwaves at zero 2D momentum are hidden ($k_0 = \pi$), while that the latter spinwaves at cSDW momenta are observable ($k_0 = 0$). Figure 1a displays $\chi_\perp(k, \omega)$ at the QCP in the observable channel, $k_0 = 0$, assuming off-diagonal magnetic frustration and a low concentration of mobile holes: $J_1^\parallel = 0$, $J_1^\perp > 0$, $J_2^\parallel = 0.3J_1^\perp = J_2^\perp$, $t_1^\parallel = -5J_1^\perp$, $t_1^\perp = 0$ and $x = 0.01$. Setting $s_0 J_1^\perp \sim 70$ meV yields a successful fit[14] to spin-wave spectra obtained from INS on the superconductor $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$ [18]. The critical spin-wave dispersion in fig. 1a also notably shows a local maximum at the Néel momentum $(\pi/a, \pi/a)$, which agrees with INS on the parent

compound CaFe_2As_2 [17]. Proximity to the QCP also naturally accounts for the low values of the magnetic moment associated with cSDW order (μ_{cSDW}) that are seen in iron-pnictide parent compounds by neutron diffraction[2]. Indeed, fig. 1b displays exact results for one hole roaming over a 4×4 square lattice of iron atoms at the QCP, where μ_{cSDW} is a fraction of the maximum possible ordered moment achieved in the true ferromagnetic state, $\mu_{\text{Fe}} = (33/31)^{1/2} 2\mu_B$. (See end of section.) Last, Eq. (5) coincides with the large- s_0 result for $\chi_{\perp}(k, \omega)$ obtained by one of the authors in the hidden ferromagnetic state at $x = 0$ [14].

The electronic structure of the hidden half-metal state can also be obtained directly from the above Schwinger-boson-slave-fermion mean field theory. In particular, the electron propagator is given by the convolution of the propagator for Schwinger bosons with the propagator for slave fermions: $iG(k, \omega) = G_b * G_f^*|_{k, \omega}$, where $iG_f(k, \omega) = \langle f(k, \omega) f^\dagger(k, \omega) \rangle$. A standard summation of Matsubara frequencies yields the expression

$$G(k, \omega) = \frac{1}{\mathcal{N}} \sum_q \left[(\cosh \theta_q)^2 \frac{n_B[\omega_b(q)] + n_F[\varepsilon_f(q - k)]}{\omega - \omega_b(q) + \varepsilon_f(q - k)} + (\sinh \theta_q)^2 \frac{n_B[\omega_b(q)] + n_F[-\varepsilon_f(q - k)]}{\omega + \omega_b(q) + \varepsilon_f(q - k)} \right]. \quad (9)$$

Ideal BEC of the Schwinger bosons at 2D momentum $\mathbf{q} = 0$ results in the following coherent contribution to the electronic spectral function at zero temperature and at large s_0 : $\text{Im } G_{\text{coh}}(k, \omega) = s_0 \pi \delta[\omega + \varepsilon_f(k)]$. It reveals the two degenerate hole bands expected from the classical picture of a half-metal state with $\nearrow_{d+} \searrow_{d-}$ spin order and with no inter-orbital hopping[14]. The fermion contribution to $\text{Im } G(k, \omega)$ above represents incoherent excitations. They show a gap Δ_{cSDW} (4) at cSDW momenta. Those originating from the second term in (9) are combinations of a hole with a spinwave, with a total energy that lies below the Fermi level. The incoherent contribution originating from the first term in (9) is the time-reversed counterpart, and it doesn't contribute at energies below the Fermi level in the zero-temperature limit. Last, the ratio of the incoherent spectral function integrated over momentum in the vicinity $\mathbf{k} = 0$ or $(\pi/a)\hat{\mathbf{x}}(\hat{\mathbf{y}})$ compared to the coherent counterpart is $\sum'_k \text{Im } G_{\text{inc}}(k, \omega) / \sum_k \text{Im } G_{\text{coh}}(k, \omega) = (\gamma/4\pi s_0) \cdot [(-\omega)\Omega_{\parallel}/(v_0/a)^2]$ as $\Delta_{\text{cSDW}} \rightarrow 0$, where $-\omega$ measures how far in energy the hole lies below the Fermi level, and where γ is the anisotropy parameter of the spinwave dispersion in question (see fig. 1a).

We will now evaluate the former incoherent contribution to the spectral function in the large- s_0 limit as $\Delta_{\text{cSDW}} \rightarrow 0$, at energies just below the Fermi level. The previous long-wavelength approximations for the spinwave dispersion near zero 2D momentum and near

cSDW momenta (6) are then valid. Also valid is the longwavelength approximation for the dispersion of the slave fermions, $\varepsilon_f(\mathbf{k}) = (2s_0)(-t_1^{\parallel})(|\mathbf{k}|^2 - k_F^2)a^2$. The imaginary part of the pole in the second term of Eq. (9) enforces energy conservation, $-\omega = \omega_b(\mathbf{q}) + \varepsilon_f(\mathbf{q} - \mathbf{k})$. The inequality $v_F > v_0$ implies diffuse electron bands centered at momenta zero and $(\pi/a)\hat{\mathbf{x}}(\hat{\mathbf{y}})$ that close out at an energy $k_F \cdot v_0/\gamma$ below the Fermi level. Figure 2 shows the net spectral function in these regions at the QCP. The incoherent contribution was evaluated in the thermodynamic limit by integrating the δ -function in energy over radial momentum analytically, and by performing the remaining angular integral numerically. Figure 2a shows that the electronic structure at zero 2D momentum is predominantly hole-type because of the coherent contribution. It is roughly consistent with the hole Fermi surface pockets about zero 2D momentum revealed by ARPES in the iron-pnictide superconductor $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$ [6][8]. (See fig. 2, caption.) Figures 2b and 2c show a mix of electron and hole structure at cSDW momentum $(\pi/a)\hat{\mathbf{x}}(\hat{\mathbf{y}})$. The “V” shape that separates pink from purple in fig. 2b and that separates purple from black in fig. 2c defines an electron Fermi velocity that coincides with the cSDW spinwave velocity along the corresponding principal axis: $v_l = v_0$ and $v_t = v_0/\gamma_{cSDW}$. ARPES measurements reported in ref. [8] also reveal electron Fermi surface pockets centered at cSDW momenta, with Fermi velocities that show the same type of anisotropy. The electron Fermi velocities extracted from the inner edge of the “V” in their dispersion curves, in particular, are $v_l \sim 0.7 \text{ \AA-eV}$ and $v_t \sim 0.3 \text{ \AA-eV}$. These values are remarkably close to the corresponding spin-wave velocities extracted from inelastic neutron scattering measurements on the same material[18]! Figures 2b and 2c also predict stronger hole dispersion at $\omega = -\varepsilon_f[\mathbf{k} - (\pi/a)\hat{\mathbf{x}}(\hat{\mathbf{y}})]$, however. It is due to the divergence of the coherence factor $\sinh^2\theta_q$ in Eq. (9) as the spin-wave frequency $\omega_b(q)$ vanishes at $\mathbf{q} = (\pi/a)\hat{\mathbf{x}}(\hat{\mathbf{y}})$. Such peaks in $\text{Im} G(k, \omega)$ must therefore disappear just off the QCP, at cSDW gaps $\Delta_{cSDW} > \Delta k_{peak} \cdot v_0$. Figures 2b and 2c yield a peak width for the hole dispersion of $\Delta k_{peak} a \sim 0.1$. The hole-dispersion peaks about cSDW momenta are therefore fragile, and they may not survive effects such as hole (slave fermion) damping and spin-wave (Schwinger boson) damping that are not accounted for within the present mean-field approximation.

We have confirmed the main results of the above mean field theory analysis of the hidden half-metal phase by obtaining the exact low-energy spectrum of one hole in the two-orbital t - J model (1) over a periodic 4×4 lattice of iron atoms using the Lanczos technique[24]. The

Hilbert space was confined to the $S_z = 1/2$ subspace, and its dimension was reduced further by exploiting translation and reflection symmetries. The Heisenberg exchange terms of the Hamiltonian (1) were stored in memory as permutations of the spin backgrounds. Hole hopping was computed at each application of the Hamiltonian (1), on the other hand. Last, the Lanczos procedure was applied numerically using the ARPACK subroutine library[25]. Figures 3a, 1b and 3b show how the magnetic order and how the low-energy spectrum of the t - J model (1) evolve with the strength of the Hund's coupling. Figure 3a displays a quantitative match between the dispersion of the exact lowest-energy spin-1/2 excitations and the prediction for spin-wave excitations about $\nearrow_{d+} \searrow_{d-}$ order at $J_0 = 0$. Next, fig. 1b shows the exact spectrum at the QCP, where degenerate groundstates exist at momenta zero and $(\pi/a)\hat{\mathbf{x}}(\hat{\mathbf{y}})$. The lowest-energy excitations again have spin 1/2, and their dispersion is qualitatively similar to the spin-wave prediction displayed by fig. 1a. This quantum-critical state shows weak cSDW order and moderate $\nearrow_{d+} \searrow_{d-}$ spin order. Last, the Hund's coupling used in fig. 1b is the critical value $-J_{0c} = 2.27J_1^\perp$. It is considerably larger than the corresponding value of $-J_{0c} = 1.35J_1^\perp$ obtained in the absence of a hole by one of the authors[14]. This is consistent with the previous mean field theory result for J_{0c} , and it is likely due to the suppression of quantum fluctuations in the antiferromagnetic state by intra-orbital hole motion. These matches indicate that the above Schwinger-boson-slave-fermion mean field theory is a valid approximation of the 2-orbital t - J model, Eq. (1), in the hidden half-metal phase. Finally, fig. 3b demonstrates that the groundstate is a robust cSDW state with a large ordered moment if Hund's rule is obeyed. It carries momentum $\pm(\pi/2a)\hat{\mathbf{x}}(\hat{\mathbf{y}})$ (cf. ref. [15]), however, and it therefore is unable to account for *any* of the Fermi surface pockets that are observed by ARPES on iron-pnictide materials[6][7][8].

III. CONCLUSIONS

Above, we have shown that a hidden half-metal state near a QCP into a cSDW state exhibits the nested 2D Fermi surfaces that are characteristic of iron-pnictide high- T_c superconductors[7][8]. The Fermi surfaces predicted here with the bare minimum of $3d_{xz}$ and $3d_{yz}$ orbitals are in fact similar to those obtained by electronic band structure calculations that include all five $3d$ orbitals[5]. In particular, zone-folded Fermi surfaces centered at momentum $(\pi/a, \pi/a)$ have low spectral weight in such case [cf. fig. 2d]. Further, our

mean field theory predicts a mixture of electron and of hole dispersion for Fermi surface pockets centered at cSDW momenta (see fig. 2). This has been observed by ARPES on iron-pnictide superconductors in certain cases[8].

We have also demonstrated above that the low-energy spectrum of the hidden half-metal state at the QCP contains zero-energy spin-wave excitations that disperse anisotropically away from cSDW momenta. The critical spin-wave spectrum notably exhibits a local maximum at the Néel momentum $(\pi/a, \pi/a)$, which is consistent with INS on a parent compound to iron-pnictide superconductors[17]. It was predicted previously by one of the authors in the case where mobile holes are absent[14]. Last, we have identified the anisotropic spin-wave velocities at cSDW momenta with the corresponding electron Fermi velocities around Fermi surface pockets centered at cSDW momenta. A comparison of independent ARPES and INS on the same iron-pnictide compound bears out this identification[8][18].

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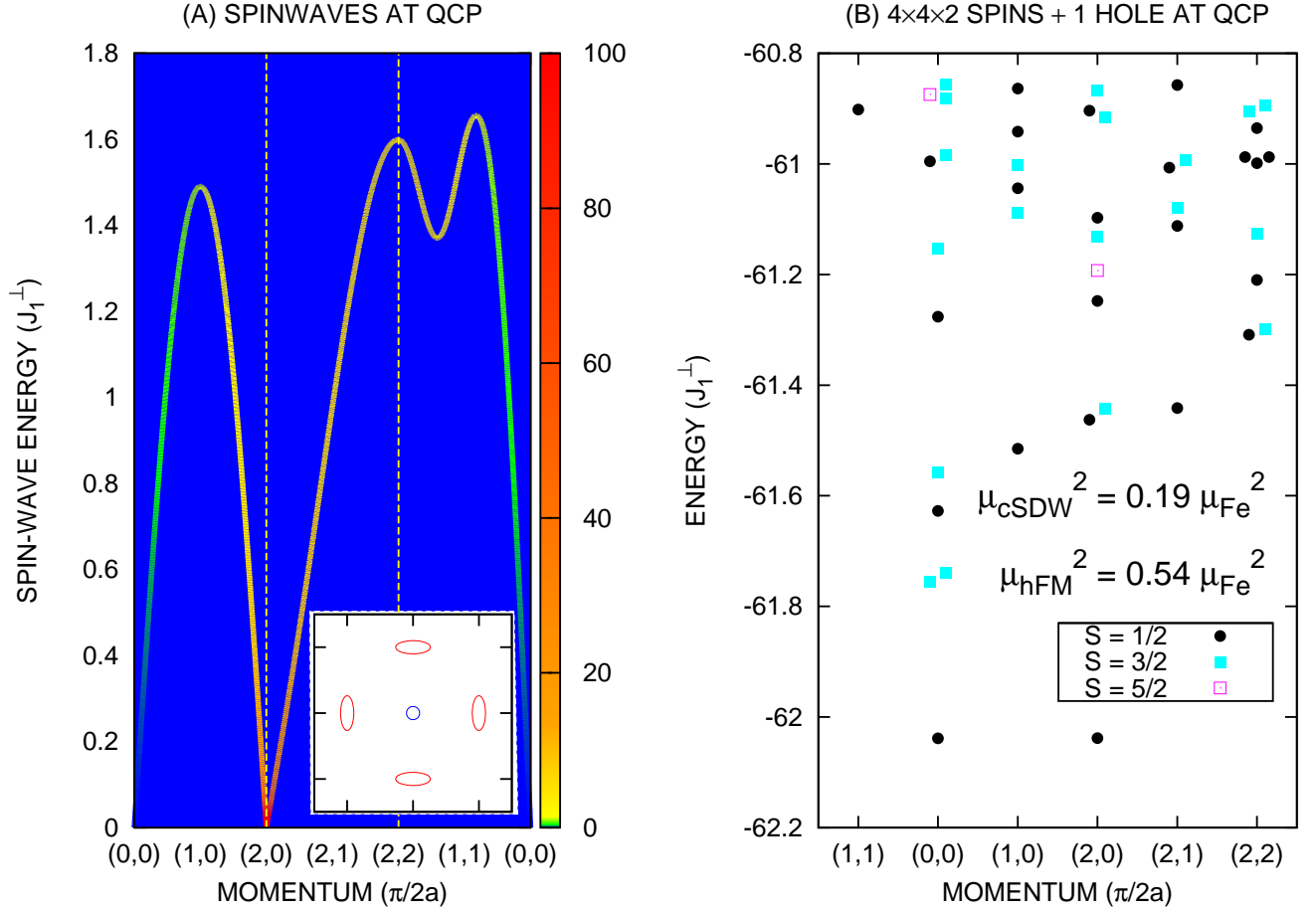


FIG. 1: The mean-field result for the dynamical spin response function in the zero-temperature-large- s_0 limit, Eq. (5), is evaluated (a) with the following set of parameters: $J_1^\parallel = 0$, $J_1^\perp > 0$, $J_2^\parallel = 0.3 J_1^\perp = J_2^\perp$, $t_1^\parallel = -5J_1^\perp$, $t_1^\perp = 0$, $x = 0.01$, $s_0 = 1/2$, and $J_0 = J_{0c}$. Low-energy contours are displayed in the inset. Also shown (b) is the low-energy spectrum of the corresponding t - J model, Eq. (1), over a $4 \times 4 \times 2$ lattice with one hole at $J_0 = -2.27 J_1^\perp$. Ordered magnetic moments over the groundstate (at zero 2D momentum) are also listed there: $\langle \boldsymbol{\mu}(k) \cdot \boldsymbol{\mu}(-k) \rangle_0$, where $\boldsymbol{\mu}(k) = [2\mu_B / (N_{\text{Fe}} - \frac{1}{2})] \sum_{\alpha=0}^1 \sum_i e^{i(k_0\alpha + \mathbf{k} \cdot \mathbf{r}_i)} \mathbf{S}_{i,\alpha}$, and where $k = (\pi, 0, 0)$ and $(0, \pi/a, 0)$, respectively, for hidden ferromagnetic (hFM) and for cSDW order. In general, $\mu_{\text{Fe}}^2 = (33/31)(2\mu_B)^2$.

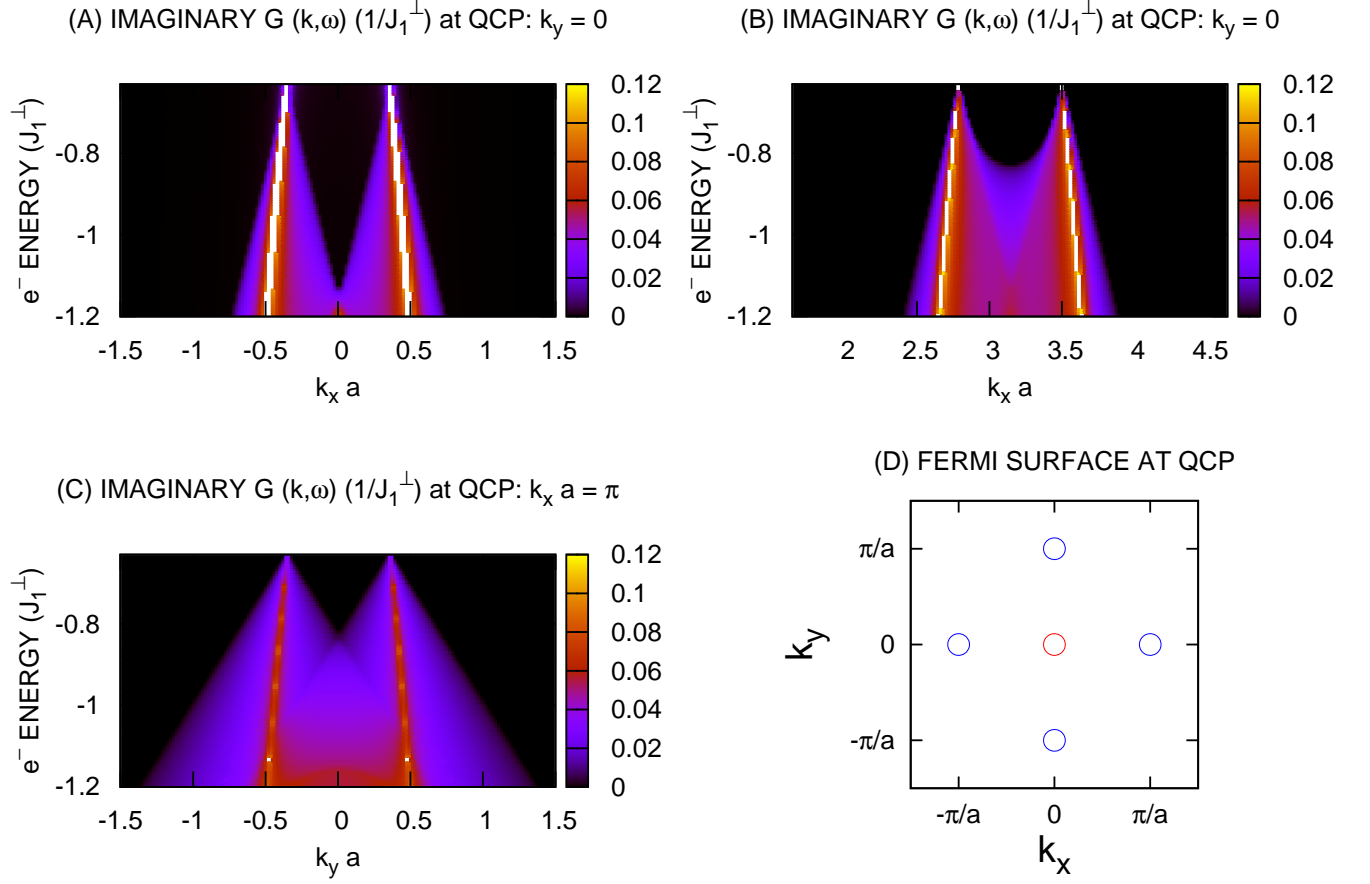


FIG. 2: Shown is the imaginary part of expression (9) with the parameter set that is listed in the previous caption, and in the following limits listed in order: $T \rightarrow 0$, then $s_0 \rightarrow \infty$, and then $\Delta_{cSDW} \rightarrow 0$. The Fe-Fe distance $a = 2.8 \text{ \AA}$ yields the Fermi momentum $k_F = 0.13 \text{ \AA}^{-1}$. Setting $s_0 J_1^\perp \sim 70 \text{ meV}$ (see text and ref. [14]) yields a spin-wave velocity $v_0 \sim 0.6 \text{ \AA-eV}$, with anisotropy parameter $\gamma_{cSDW} = 2.64$, and a Fermi velocity $v_F \sim 1.4 \text{ \AA-eV}$. Also shown are the Fermi surfaces predicted by Eq. (9). Each is doubly degenerate because of the $3d_{xz}$ and $3d_{yz}$ orbitals.

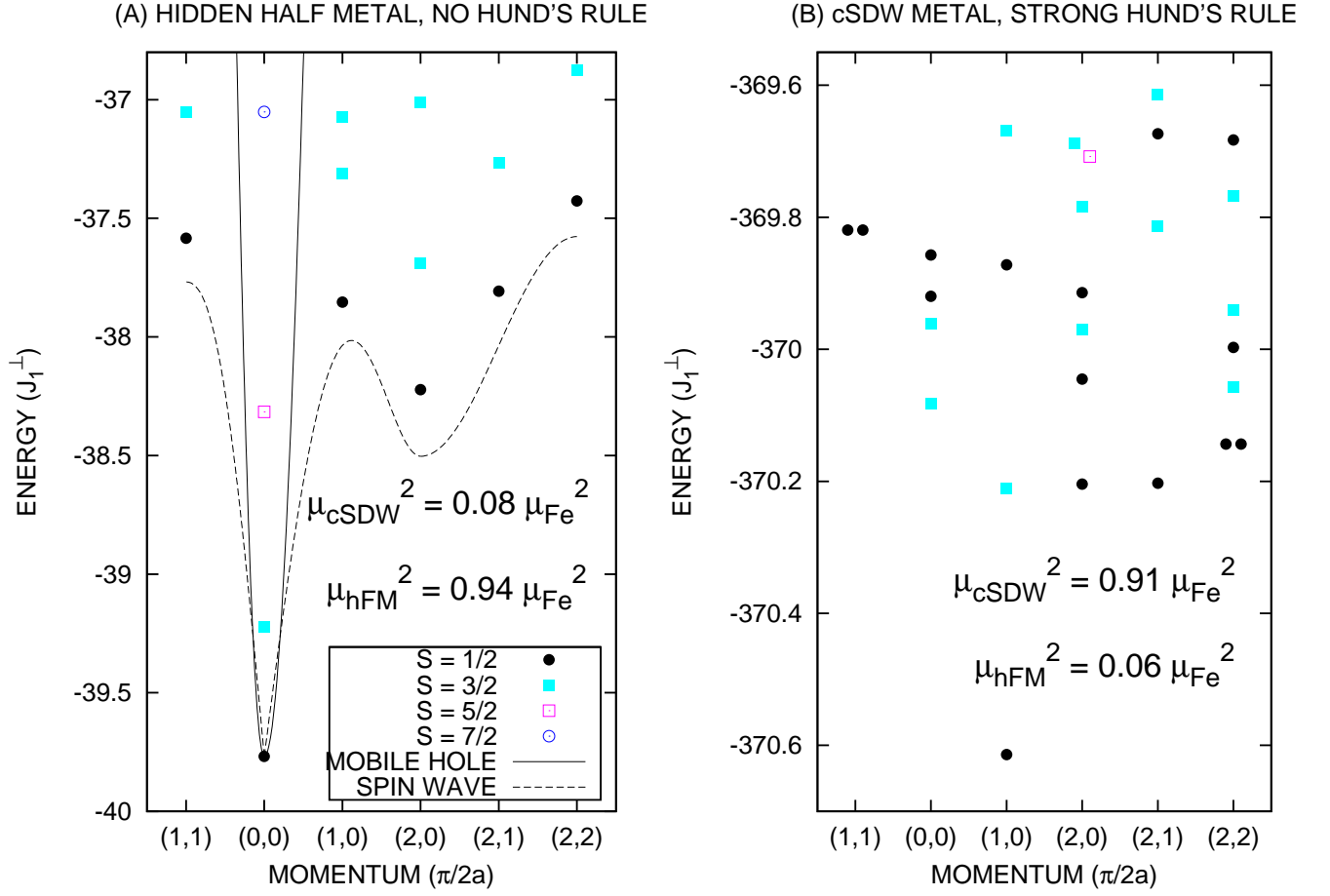


FIG. 3: Shown are low-energy spectra of the t - J model, Eq. (1), over a $4 \times 4 \times 2$ lattice with one hole, with the parameters listed in the text. Each point is doubly degenerate because $t_1^\perp = 0$. A comparison with the hole spectrum, $\varepsilon_f(k)$, and with the spin-wave spectrum, $\omega_b(k)$, is made (a) at $x = 0$ in the absence of Hund's rule, $J_0 = 0$. The latter is enforced (b) by setting $J_0 = -23 J_1^\perp$.